Bayesian Methods

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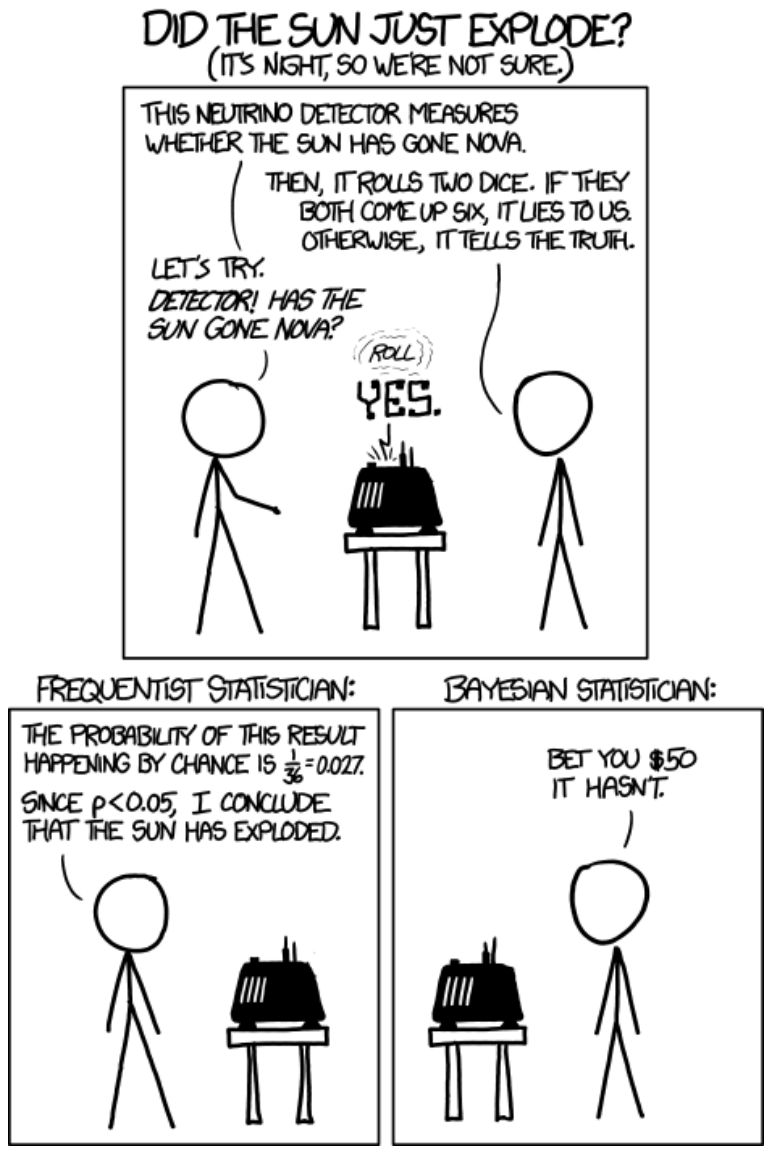
Where Are We Heading to?

How to build good ML models

- Making use of a crowd ⇒ Week 7 Ensemble methods
  each of us is a biological prediction model trained on different datasets...
- Using a neural network ⇒ Week 8 and 9 Neural networks
  brain-inspired models, some are good for images...
- Making a robust model ⇒ Week 10 Robust machine learning
  malicious users, outliers,...
- Asking for explanations ⇒ Week 11 Interpretable machine learning
  ...let's ask the machines for explanations...
- Exploiting prior beliefs ⇒ Week 12 Bayesian methods

Frequentist vs Bayesian



- We are often interested in learning probabilistic models of a given dataset
  - a probabilistic model describes a probabilistic process that generates the data
  - e.g. Gaussian distributions form a class of probabilistic model for real-valued observations
- The frequentist approach picks a probabilistic model that best fits the dataset
  - e.g., naive Bayes classifier
- The Bayesian approach assigns a weight to each candidate probabilistic model by using the Bayes' rule to combine
  - prior subjective assessment on how likely the model is, and
  - how well the model explains the dataset.

Bayesian Learning

Frequentist learning

- Suppose we have a dataset D, and we have a family of probabilistic models $\{p(\cdot \mid \theta) : \theta \in \Theta\}$, where θ is the parameter vector of $p(D \mid \theta)$, and Θ is the parameter space.
- In the frequentist approach, we often learn a single model $p(\cdot \mid \theta)$ by maximizing the likelihood

$$\max_{\theta} p(D \mid \theta),$$

  where $p(D \mid \theta)$ is the probability that D is generated by the model $p(\cdot \mid \theta)$, and often called the likelihood.
- The likelihood is a measure of the compatibility between the model θ and the data D.

Bayes' Theorem (aka Bayes' law or Bayes' rule)

- For two events A and B, if $P(B) \neq 0$, then

$$P(A \mid B) = \frac{P(B \mid A)P(A)}{P(B)}.$$

- Interpretation
  - B: the observation/evidence
  - $P(A)$: the prior, or the initial belief for A
  - $P(B \mid A)$: the likelihood
  - $P(A \mid B)$: the posterior, or the belief for A after observing B

Bayesian learning

- In the Bayesian approach, instead of learning a single model, we learn a distribution on all the models in Θ.
- Specifically, we assume a prior distribution $p(\theta)$ on Θ, and given a dataset D, we compute a posterior

$$\overbrace{p(\theta \mid D)}^{\text{posterior}} = p(\theta)p(D \mid \theta)/Z \propto \overbrace{p(\theta)}^{\text{prior}}\overbrace{p(D \mid \theta)}^{\text{likelihood}},$$

  where the normalization constant Z is

$$Z = \begin{cases} \sum_{\theta \in \Theta} p(\theta)p(D \mid \theta), & \text{if } p(\theta) \text{ is discrete,} \\ \int_{\Theta} p(\theta)p(D \mid \theta)d\theta, & \text{if } p(\theta) \text{ is continuous.} \end{cases}.$$

- The posterior distribution $p(\theta \mid D)$ can be used in various ways when performing inference.

Inference problems

- Compute the MAP (maximum a posterior) model:

$$\theta_{\text{MAP}} = \operatorname*{argmax}_{\theta \in \Theta} p(\theta \mid D).$$

- Compute the (posterior) predictive distribution:

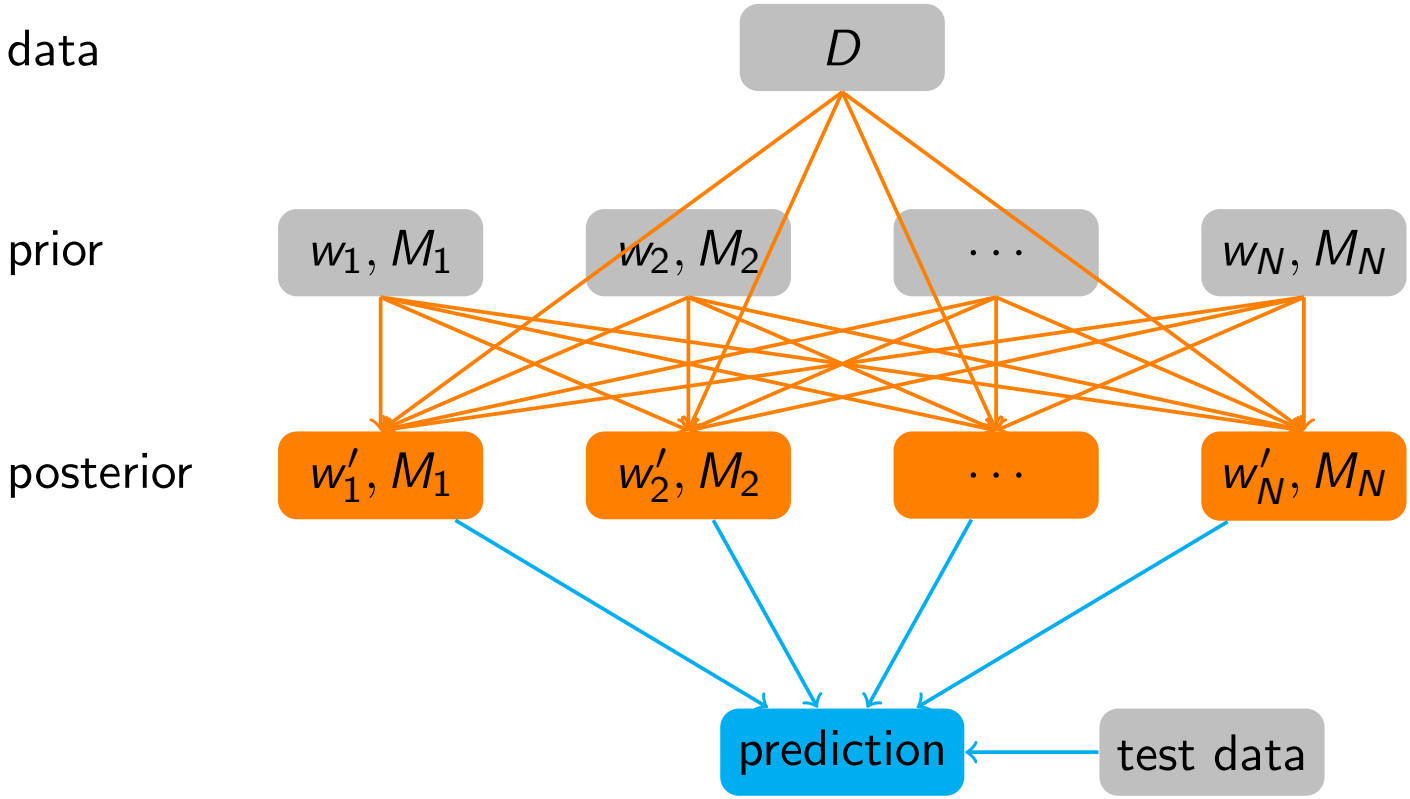
$$p(y \mid D, x) = \int p(y \mid \theta, x) p(\theta \mid D) d\theta.$$

- Compute posterior mean and variance of Y given x:

$$\text{posterior mean } \mu_x = \mathbb{E}(Y \mid x, D) = \int y p(y \mid D, x) dy$$

$$\text{posterior variance } \sigma_x^2 = \text{Var}(Y \mid x, D) = \int (y - \mu_x)^2 p(y \mid D, x) dy$$

Bayesian method as an ensemble method



- Learning (computing posterior): construct a weighted ensemble of (often infinitely many) models using the Bayes' rule .
- Prediction: aggregate the ensemble's predictions (e.g., by computing the weighted average prediction).

Example. Learning the probability of Heads

- Peter has two coins: the probability of Heads for one is 0.5, and 0.8 for the other. He chooses a coin, tosses it twice and observes one Head and one Tail. What's the probability of Heads of the chosen coin?
- The parameter space is $\Theta = \{0.5, 0.8\}$, the dataset D is a sequence of two Heads, and the likelihood is

$$p(D \mid \theta) = \theta(1 - \theta).$$

The frequentist solution

- We have

$$p(D \mid \theta = 0.5) = 0.25,$$
$$p(D \mid \theta = 0.8) = 0.16.$$

- Thus $\theta = 0.5$ is more compatible with the observations, and we may believe that the probability of Heads for the chosen coin is 0.5.

The Bayesian solution

- We heard from a close friend of Peter that he likes the biased coin and chooses it with probability 0.9, that is, our prior is $p(\theta = 0.5) = 0.1$ and $p(\theta = 0.8) = 0.9$.
- We have $p(\theta = 0.5)p(D \mid \theta = 0.5) = 0.025$, and $p(\theta = 0.8)p(D \mid \theta = 0.8) = 0.144$, thus the posterior distribution is

$$p(\theta \mid D) = \begin{cases} 25/169 & \theta = 0.5 \\ 144/169 & \theta = 0.8. \end{cases}$$

The MAP model is $\theta = 0.8$, thus we may believe that the probability of Heads for the chosen coin is 0.8.

- The posterior mean of θ is $0.5 \times 25/169 + 0.8 \times 144/169 = 0.76$. The standard deviation of θ given D is 0.18 (exercise).
- The probability distribution of the outcomes of next two tosses is

outcome	HH	HT	TH	TT
p	0.5823	0.1733	0.1733	0.0711

Bayesian regression and classification

- In Bayesian regression and classification methods,
  - the probabilistic model $p(D \mid \theta)$ is often much more complex than a simple Bernoulli distribution, and
  - the prior $p(\theta)$ is much more complex than a discrete distribution.
- Two challenges
  - Specifying a good prior can be hard.
  - The inference problems are often computationally hard.
- We focus on the Gaussian processes, which
  - support a wide range of priors on all possible functions,
  - allow elegant algorithms for the inference problems.

From SVM to Gaussian Process

Support vector regression

- Recall: in binary support vector classifier, the discriminant function is of the form

$$f(\mathbf{x}) = \sum_i \alpha_i y_i k(\mathbf{x}_i, \mathbf{x}).$$

  $\mathbf{x}$ is predicted to be positive if $f(\mathbf{x}) > 0$ and negative otherwise.
- SVMs can be used for regression too, and the regressor is of the form

$$f(\mathbf{x}) = \sum_i \alpha_i k(\mathbf{x}_i, \mathbf{x}).$$

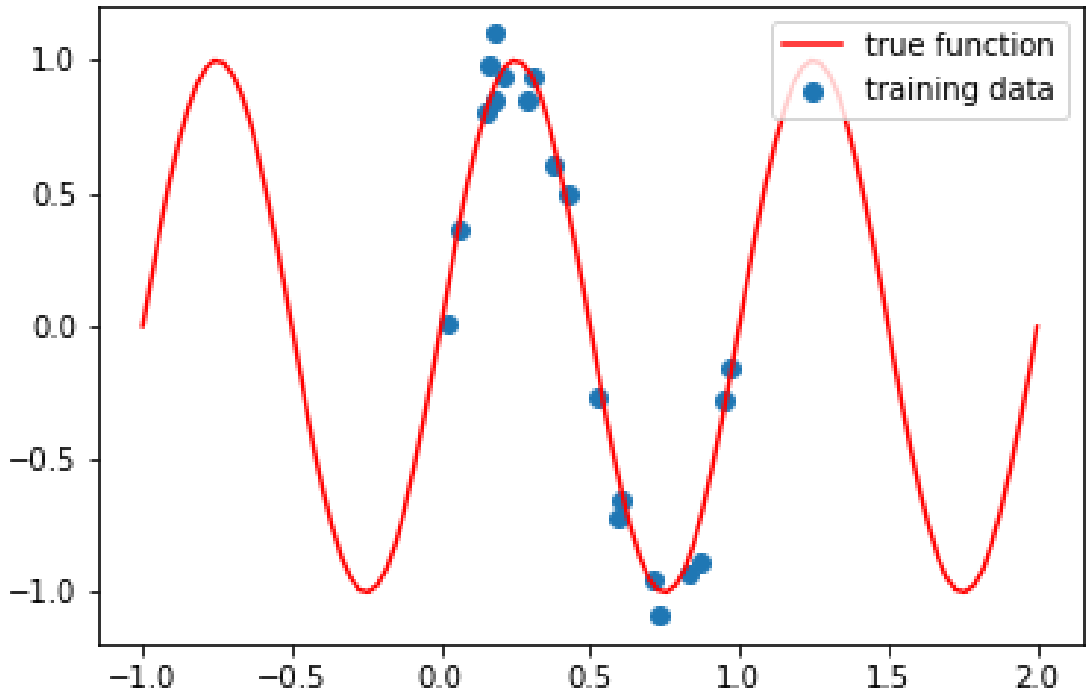
Gaussian processes (GPs)

- Gaussian processes also produce regression estimates of the same form as SVMs:

$$f(\mathbf{x}) = \sum_i \alpha_i k(\mathbf{x}_i, \mathbf{x}).$$

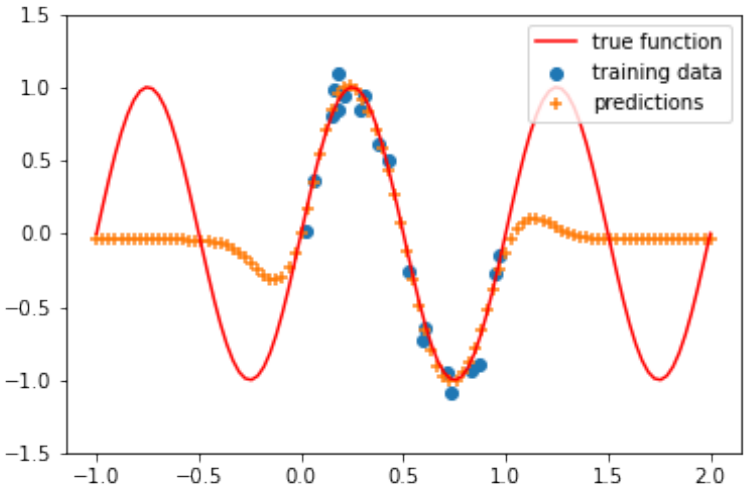
- However, there are a few important differences
  - SVM predicts a single estimated value, but GP predicts a distribution on the possible values.
  - in SVM, the kernel hyperparameters are often tuned by using methods like cross validation to choose the best values from a small set of candidate values; in GP, the hyperparameters can be optimized over all possible values using numerical optimization methods.

Example. Learning the sine function

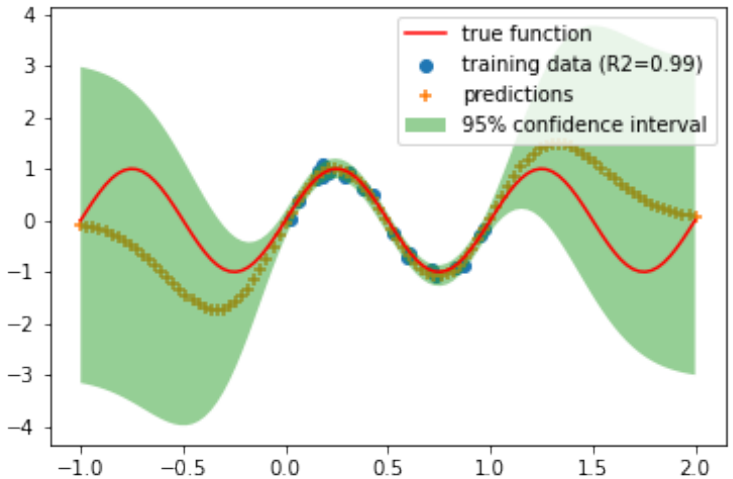


- $Y = \sin(2\pi x) + \epsilon$, where $\epsilon \sim N(0, 0.1^2)$.
- Training set: x sampled from [0, 1]
- Prediction: x sampled from [-1, 2]

  $\Rightarrow$ we can observe how well an algorithm interpolates and extrapolates.



SVM (RBF kernel with $\gamma = 2000$)



Gaussian process (RBF kernel)

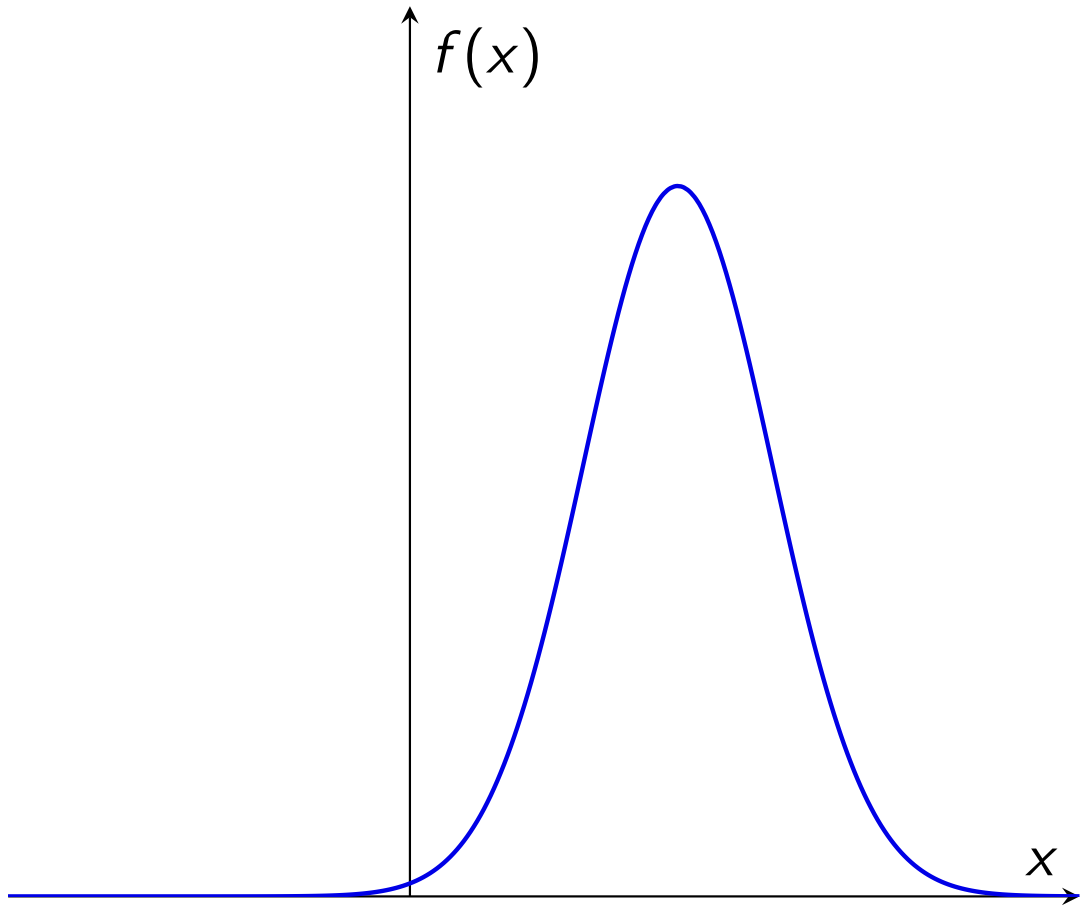
Gaussian Distributions ~~101~~ 102

Univariate Gaussian distribution

- A random variable Y is said to follow a univariate Gaussian distribution $N(\mu, \sigma^2)$ if its probability density function (PDF) is

$$f(y) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(y-\mu)^2}{2\sigma^2}\right). \tag{1}$$

- We often write this as $Y \sim N(\mu, \sigma^2)$, and use $N(y; \mu, \sigma^2)$ to denote the PDF.



PDF of a Gaussian distribution

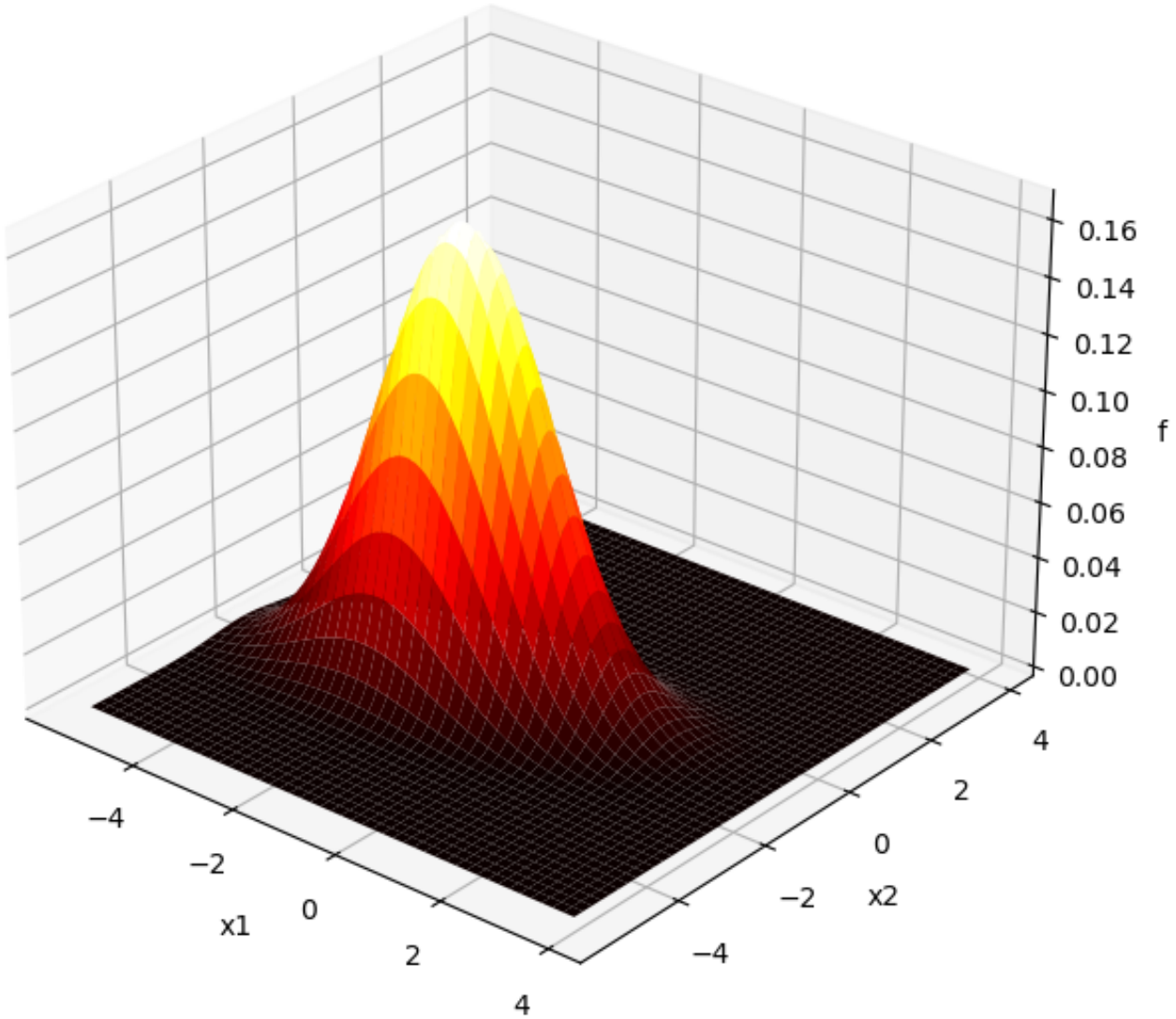
Multivariate Gaussian distribution

- A random vector $\boldsymbol{Y} = (Y_1, \ldots, Y_n)^\top$ is said to follow a multivariate Gaussian distribution $N(\boldsymbol{\mu}, \Sigma)$ with mean $\boldsymbol{\mu}$ and covariance matrix Σ if its PDF is

$$f(\mathbf{y}) = \frac{1}{\sqrt{|2\pi\Sigma|}} \exp\left(-\frac{1}{2}(\mathbf{y}-\boldsymbol{\mu})^\top \Sigma^{-1}(\mathbf{y}-\boldsymbol{\mu})\right), \tag{2}$$

  where we use the notation $|A|$ to denote the determinant of a matrix A.

- We often write this as $\boldsymbol{Y} \sim N(\boldsymbol{\mu}, \Sigma)$, and use $N(\mathbf{y}; \boldsymbol{\mu}, \Sigma)$ to denote the PDF.



PDF of a bivariate Gaussian

- Notations: Let $I = \{i_1, i_2, \ldots, i_k\}$ and $J = \{j_1, \ldots, j_l\}$ be ordered sets/sequences. Then x_I denotes $(x_{i_1}, \ldots, x_{i_k})^\top$, and Σ_{IJ} denotes $\begin{pmatrix} \sigma_{i_1 j_1} & \sigma_{i_1 j_2} & \ldots & \sigma_{i_1 j_1} \\ & & \ldots & \\ \sigma_{i_k j_1} & \sigma_{i_k j_2} & \ldots & \sigma_{i_k j_l} \end{pmatrix}$, where σ_{ij} is the (i,j)th element of Σ.

Marginal distribution

- The marginal distribution of a Gaussian distribution is also a Gaussian distribution.
- Specifically, we partition $\{1, \ldots, d\}$ into two disjoint subsets I_1 and I_2 with n_1 and n_2 elements respectively, and let

$$\boldsymbol{Y}_i = Y_{I_i}, \qquad \boldsymbol{\mu}_i = \boldsymbol{\mu}_{I_i}, \qquad \Sigma_{ij} = \Sigma_{I_i I_j}.$$

- Then the marginal distribution of $\boldsymbol{Y}_1$ is

$$f_1(\mathbf{y}_1) = N(\mathbf{y}_1; \boldsymbol{\mu}_1, \Sigma_{11}). \tag{3}$$

Conditional distribution

- The conditional distribution of a Gaussian distribution is also a Gaussian distribution.
- Specifically, the distribution of $\boldsymbol{Y}_2$ given $\boldsymbol{Y}_1 = \mathbf{y}_1$ is

$$f_{2|1}(\mathbf{y}_2|\mathbf{y}_1) = N(\mathbf{y}_2; \boldsymbol{\mu}_2 + \Sigma_{21}\Sigma_{11}^{-1}(\mathbf{y}_1 - \boldsymbol{\mu}_1), \Sigma_{22} - \Sigma_{21}\Sigma_{11}^{-1}\Sigma_{12}). \quad (4)$$

- We often drop the subscripts in f_1 and $f_{2|1}$ when there is no confusion.

Example. Bivariate Gaussian

- Let Y_1 and Y_2 be the returns for two investments. They are known to have a joint distribution

$$\begin{pmatrix} Y_1 \\ Y_2 \end{pmatrix} \sim N\left(\begin{pmatrix} -1 \\ -2 \end{pmatrix}, \begin{pmatrix} 1 & 2 \\ 2 & 5 \end{pmatrix} \right).$$

- Then the marginal distributions are

$$Y_1 \sim N(-1, 1), \qquad\qquad Y_2 \sim N(-2, 5).$$

- The conditional distribution of Y_1 given $Y_2 = 3$ has mean $-1 + 2 \cdot \frac{1}{5} \cdot (3 - (-2)) = 1$ and variance $1 - 2 \cdot \frac{1}{5} \cdot 2 = \frac{1}{5}$, that is,

$$Y_1 \mid Y_1 = 3 \sim N(1, 1/5).$$

  The conditional distribution of Y_2 given $Y_1 = 2$ has mean $-2 + 2 \cdot \frac{1}{1} \cdot (2 - (-1)) = 4$ and variance $5 - 2 \cdot \frac{1}{1} \cdot 2 = 1$, that is,

$$Y_2 \mid Y_1 = 2 \sim N(4, 1).$$

Example. Trivariate Gaussian

- Let Y_1, Y_2, Y_3 be the returns for three investments. They are known to have a joint distribution

$$\begin{pmatrix} Y_1 \\ Y_2 \\ Y_3 \end{pmatrix} \sim N\left(\begin{pmatrix} -1 \\ -2 \\ 1 \end{pmatrix}, \begin{pmatrix} 1 & 2 & 1 \\ 2 & 5 & 2 \\ 1 & 2 & 4 \end{pmatrix} \right).$$

- The conditional distribution of Y_1, Y_2 given $Y_3 = 2$ has mean $\begin{pmatrix} -1 \\ -2 \end{pmatrix} + \begin{pmatrix} 1 \\ 2 \end{pmatrix} (4)^{-1}(2-1) = \begin{pmatrix} -3/4 \\ -3/2 \end{pmatrix}$, and covariance matrix $\begin{pmatrix} 1 & 2 \\ 2 & 5 \end{pmatrix} - \begin{pmatrix} 1 \\ 2 \end{pmatrix} (4)^{-1} \begin{pmatrix} 1 & 2 \end{pmatrix} = \begin{pmatrix} 3/4 & 3/2 \\ 3/2 & 4 \end{pmatrix}$, thus

$$\begin{pmatrix} Y_1 \\ Y_2 \end{pmatrix} \Big| Y_3 = 2 \sim N\left(\begin{pmatrix} -3/4 \\ -3/2 \end{pmatrix}, \begin{pmatrix} 3/4 & 3/2 \\ 3/2 & 4 \end{pmatrix} \right)$$

Gaussian Processes (GPs)

A generalization of multivariate Gaussians

- Specifically, a Gaussian process (GP) is a collection of random variables such that any finite subset of which follows a (multivariate) Gaussian distribution.
- Recall: if $(Y_1, \ldots, Y_n)$ follows a multivariate Gaussian distribution, then any subset of them follows a multivariate Gaussian distribution.

  $\Rightarrow$ a multivariate Gaussian distribution is a GP.

Mean and kernel

- A GP can be specified in terms of the mean function m and the covariance function (aka kernel) k, defined by

$$m(Y) = \mathbb{E}(Y),$$
$$k(Y, Y') = \mathrm{cov}(Y, Y'),$$

  where Y and Y' are any two random variables in the GP

- For example, if the GP under consideration is a multivariate Gaussian $\boldsymbol{Y} = (Y_1, \ldots, Y_n)^\top \sim N(\boldsymbol{\mu}, \Sigma)$, then

$$m(Y_i) = \mu_i,$$
$$k(Y_i, Y_j) = \sigma_{ij}.$$

GPs as Distributions on Functions

- In many cases, each random variable in a GP can be considered as the output on an input.
- In particular, we often consider a GP $\{Y(\mathbf{x}) : \mathbf{x} \in \mathbf{R}^d\}$, where $\mathbf{x}$ denotes an input feature vector, and $Y(\mathbf{x})$ denotes the output for $\mathbf{x}$.
- If we define a random function F such that $F(\mathbf{x})$ is $Y(\mathbf{x})$, then the GP is the probability distribution for F, and we write

$$F \sim GP(m, k),$$

where m and k are the mean function and the covariance function of the GP.

- For example, consider $Y \sim N(\mu, \sigma^2)$. This can be viewed as a distribution of real-valued functions defined on a set $\{\mathbf{x}_1\}$ with a single feature vector, where the PDF of a function f defined on $\{\mathbf{x}_1\}$ is

$$p(f) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(f(\mathbf{x}_1)-\mu)^2}{2\sigma^2}}.$$

- Similarly, if $\boldsymbol{Y} = (Y_1, \ldots, Y_n)^\top \sim N(\boldsymbol{\mu}, \Sigma)$, then it can be viewed as a distribution of real-valued functions defined on n feature vectors $\{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$.

- The covariance function $k(Y(\mathbf{x}), Y(\mathbf{x}'))$ is then a function of $\mathbf{x}$ and $\mathbf{x}'$ and often simply written as $k(\mathbf{x}, \mathbf{x}')$.
- Intuitively, the kernel controls how the outputs for $\mathbf{x}$ and $\mathbf{x}'$ are related with each other.
- As in SVMs, the choice of the kernel is important in GPs.

GP Regression

Noise-free observation model

- Consider a training set $D = (\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n) \in \mathbf{R}^d \times \mathbf{R}$.
- In the noise-free GP model, we assume that D is generated as follows
  - sample f from $GP(m, k)$,
  - for each input $\mathbf{x}_1, \ldots, \mathbf{x}_n$, observe

$$y_i = f(\mathbf{x}_i).$$

- We want to make predictions on $\mathbf{x}'_1, \ldots, \mathbf{x}'_t$.
- Note: we assume $\mathbf{x}_i$'s and $\mathbf{x}'_i$'s are all different.

- Notations

notation	meaning
$\mathbf{X}$	matrix with $\mathbf{x}_i^\top$ as the ith row
$\mathbf{X}'$	matrix with $\mathbf{x}_i'^\top$ as the ith row
$\mu_{\mathbf{X}}$	$(m(\mathbf{x}_1), \ldots, m(\mathbf{x}_n)^\top$; $\mu_{\mathbf{X}'}$ similarly defined
$\boldsymbol{Y}$	$(Y(\mathbf{x}_1), \ldots, Y(\mathbf{x}_n))^\top$
$\mathbf{y}$	$(y_1, \ldots, y_n)^\top$
$\boldsymbol{Y}'$	$(Y(\mathbf{x}_1'), \ldots, Y(\mathbf{x}_t'))^\top$
$K_{\mathbf{X},\mathbf{X}'}$	matrix with $k(\mathbf{x}_i, \mathbf{x}_j')$ as the (i,j)th entry
	here $\mathbf{X}$ *and* $\mathbf{X}'$ *can be any two matrices*

Prediction

- The joint distribution of $\boldsymbol{Y}$ and $\boldsymbol{Y}'$ is

$$\begin{pmatrix} \boldsymbol{Y} \\ \boldsymbol{Y}' \end{pmatrix} \sim N\left(\begin{pmatrix} \mu_{\mathbf{X}} \\ \mu_{\mathbf{X}'} \end{pmatrix}, \begin{pmatrix} K_{\mathbf{X},\mathbf{X}} & K_{\mathbf{X},\mathbf{X}'} \\ K_{\mathbf{X}',\mathbf{X}} & K_{\mathbf{X}',\mathbf{X}'} \end{pmatrix} \right).$$

- The predictive distribution of $\boldsymbol{Y}'$ is

$$\boldsymbol{Y}' \mid \mathbf{X}', \mathbf{X}, \mathbf{y} \sim N\Big(\overbrace{\underset{t\times 1}{\mu_{\mathbf{X}'}} + \underset{t\times n}{K_{\mathbf{X}',\mathbf{X}}} \underset{n\times n}{K_{\mathbf{X},\mathbf{X}}^{-1}} \underset{n\times 1}{(\mathbf{y} - \mu_{\mathbf{X}})}}^{\text{posterior mean}}, \tag{5}$$

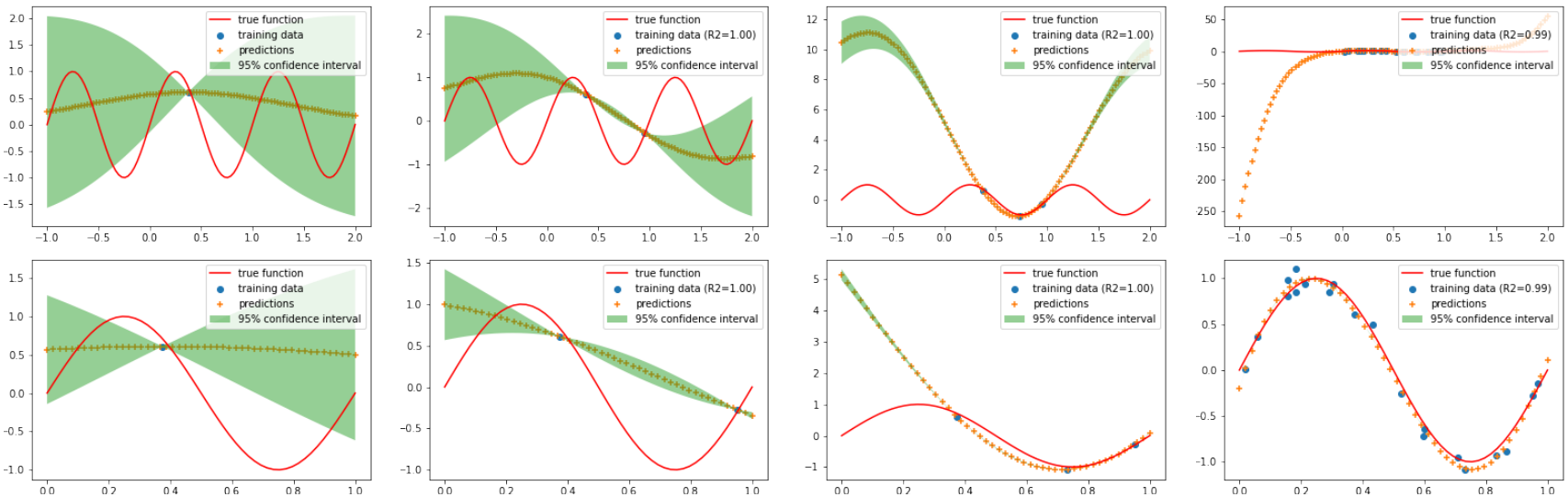
$$\overbrace{\underset{t\times t}{K_{\mathbf{X}',\mathbf{X}'}} - \underset{t\times n}{K_{\mathbf{X}',\mathbf{X}}} \underset{n\times n}{K_{\mathbf{X},\mathbf{X}}^{-1}} \underset{n\times t}{K_{\mathbf{X},\mathbf{X}'}}}^{\text{posterior covariance}} \Big). \tag{6}$$

- Let $(\alpha_1, \ldots, \alpha_n)^\top = K_{\mathbf{X},\mathbf{X}}^{-1}(\mathbf{y} - \mu_{\mathbf{X}})$, then for any $\mathbf{x}'$, its posterior mean is

$$f(\mathbf{x}') = \mu_{\mathbf{x}'} + \sum_{i=1}^{n} \alpha_i k(\mathbf{x}', \mathbf{x}_i).$$

Evolution of noise-free GP with $m = 0$ and $k(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{\|\mathbf{x}-\mathbf{x}'\|^2}{2}\right)$

$n = 1$ $n = 2$ $n = 3$ $n = 20$



- Good training set performance with all training set R^2 values nearly 1.
- Interpolation performance improves as n increases, but extrapolation performance becomes worse; in addition uncertainty estimates are often nearly 0 and not useful.

Noisy observation model

- In general, the observed value y is only a noisy observation of the true value.
- The noisy observation model is the same as the noise-free model, except that y_i is not $f(\mathbf{x}_i)$, but

$$y = f(\mathbf{x}) + \epsilon,$$

where $\epsilon \sim N(0, \sigma^2)$, and σ^2 is an unknown constant.

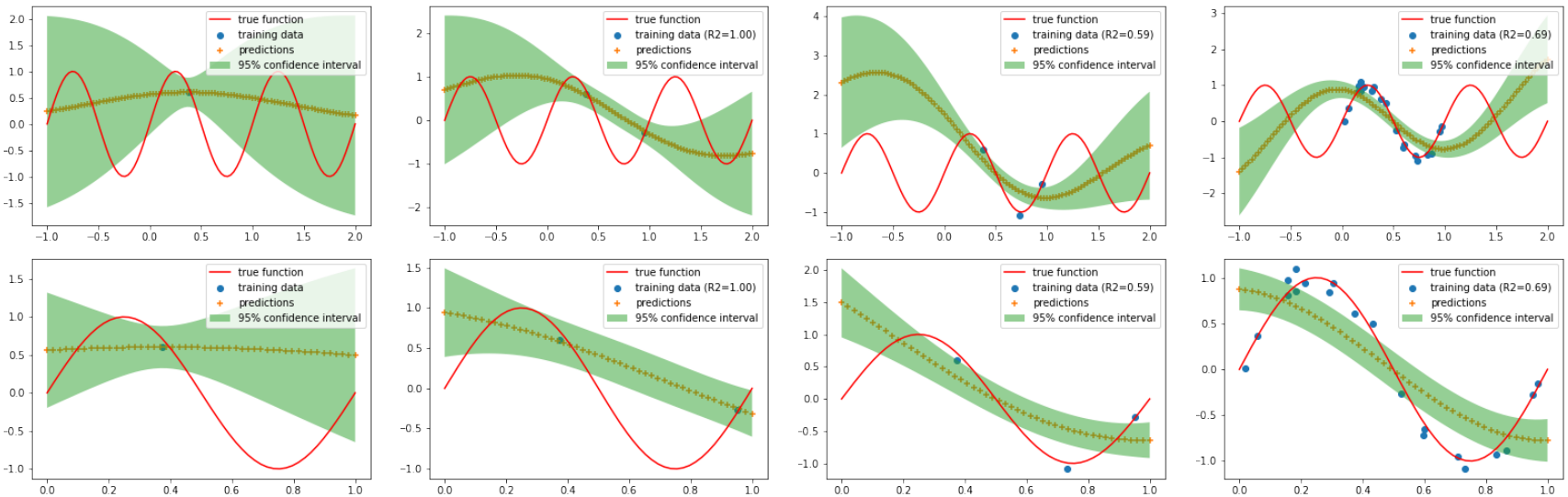
- The predictive distribution is

$$\boldsymbol{Y}' \mid \mathbf{X}', \mathbf{X}, \mathbf{y} \sim N\Big(\overbrace{\underset{t\times 1}{\mu_{\mathbf{X}'}} + \underset{t\times n}{K_{\mathbf{X}',\mathbf{X}}}\underset{n\times n}{(K_{\mathbf{X},\mathbf{X}} + \sigma^2 I)^{-1}}\underset{n\times 1}{(\mathbf{y} - \mu_{\mathbf{X}})}}^{\text{posterior mean}}, \tag{7}$$

$$\overbrace{\underset{t\times t}{K_{\mathbf{X}',\mathbf{X}'}} - \underset{t\times n}{K_{\mathbf{X}',\mathbf{X}}}\underset{n\times n}{(K_{\mathbf{X},\mathbf{X}} + \sigma^2 I)^{-1}}\underset{n\times t}{K_{\mathbf{X},\mathbf{X}'}}}^{\text{posterior covariance}}\Big). \tag{8}$$

Evolution of noisy GP with $m = 0$, $k(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{\|\mathbf{x}-\mathbf{x}'\|^2}{2}\right)$ and $\sigma^2 = 0.01$.

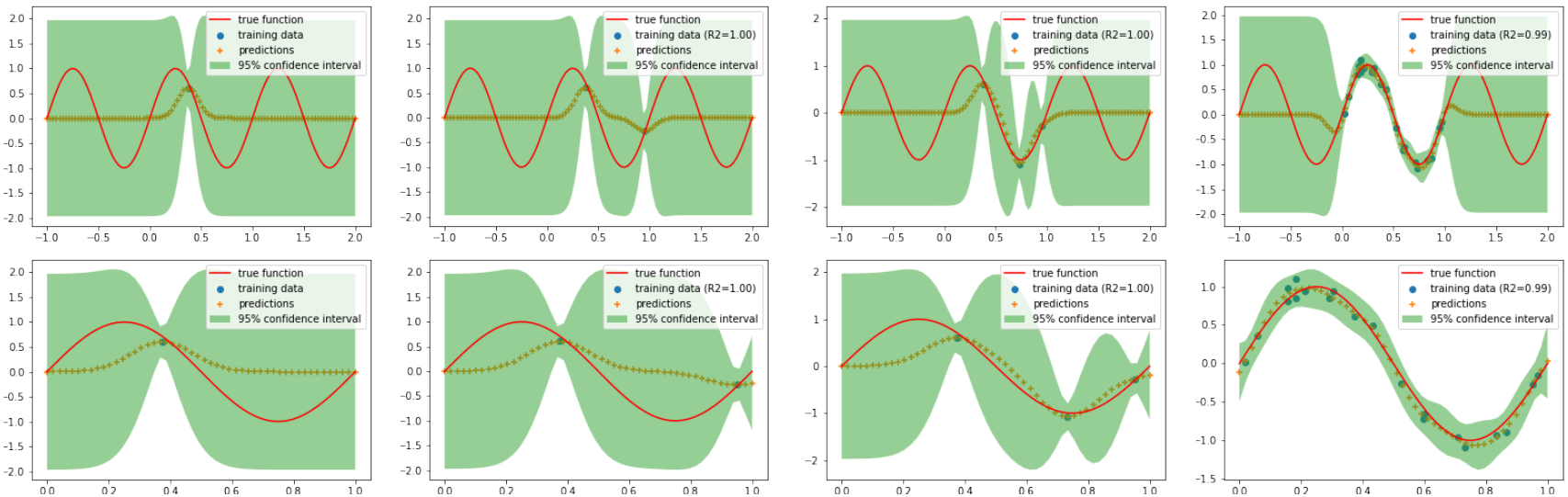
$n = 1$ $n = 2$ $n = 3$ $n = 20$



- Incorporating noise in the observation leads to weaker training set performance, but better confidence intervals and better extrapolation performance.

Evolution of noisy GP with $m = 0$, $k(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{\|\mathbf{x}-\mathbf{x}'\|^2}{0.02}\right)$ and $\sigma^2 = 0.01$.

$n = 1$ $n = 2$ $n = 3$ $n = 20$



- Using an RBF kernel with a smaller length scale leads to good interpolation and extrapolation performance; and the uncertainty estimates are good, though slightly too large.

  Question: Can we learn σ^2 and other hyperparameters from data?

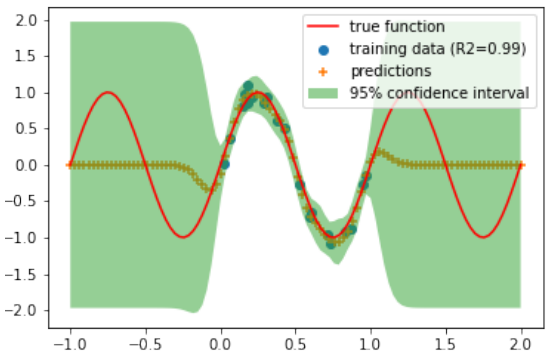
Model Selection

- The problem of choosing the hyperparameters of a GP model is a problem of model selection, thus we can use techniques such as cross-valiation.
- Let φ be the learnable parameters of the mean function m and the kernel function k, and the observation noise variance σ^2. We can choose φ by maximizing the likelihood function

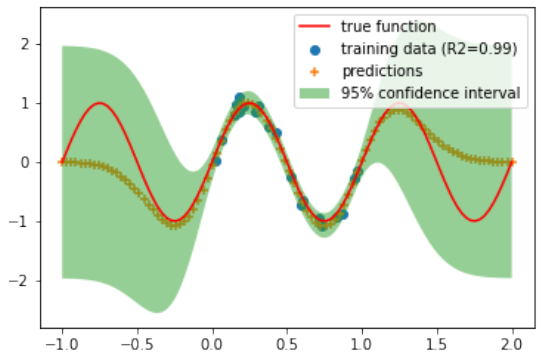
$$L(\varphi) = p(\mathbf{y} \mid \mathbf{X}, m, k) = N(\mathbf{y}; \mu_{\mathbf{X}}, K_{\mathbf{X},\mathbf{X}}). \tag{9}$$

- The likelihood function measures the compability between φ and the data.
- Various numerical optimization algorithms can be used to maximize the likelihod function (details beyond this course).

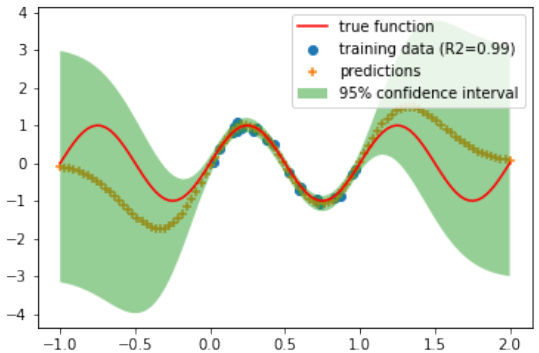
Scaled RBF kernel $c \exp(-(\mathbf{x} - \mathbf{x}')^2/(2\ell^2))$, $m = 0$



$c = 1, \ell = 0.1, \sigma^2 = 0.01$



$c = 1, \ell = 0.335, \sigma^2 = 0.00821$



$c = 2.435, \ell = 0.335, \sigma^2 = 0.00821$

Hyperparameters in red are learned.

Commonly-used Kernels

- Not every function $k(\mathbf{x}, \mathbf{x}')$ can be used as a kernel function in SVMs; this is true in GPs too.
- Using the right kernel is often important to make GPs work.
- In practice, we can try commonly used kernels, or try kernels constructed using them.

Constant kernel

- The constant kernel is defined as

$$k(\mathbf{x}, \mathbf{x}') = c, \tag{10}$$

  where $c \geq 0$ is a constant.
- This is not really an interesting kernel on its own, but is useful when constructing new kernels using known kernels.

Linear kernel

- The linear kernel is defined as

$$k_{\text{linear}}(\mathbf{x}, \mathbf{x}') = \mathbf{x}^\top \mathbf{x}' + \sigma_0^2.$$

  The linear kernel is said to be homogeneous is $\sigma_0 = 0$ and inhomogeneous otherwise.

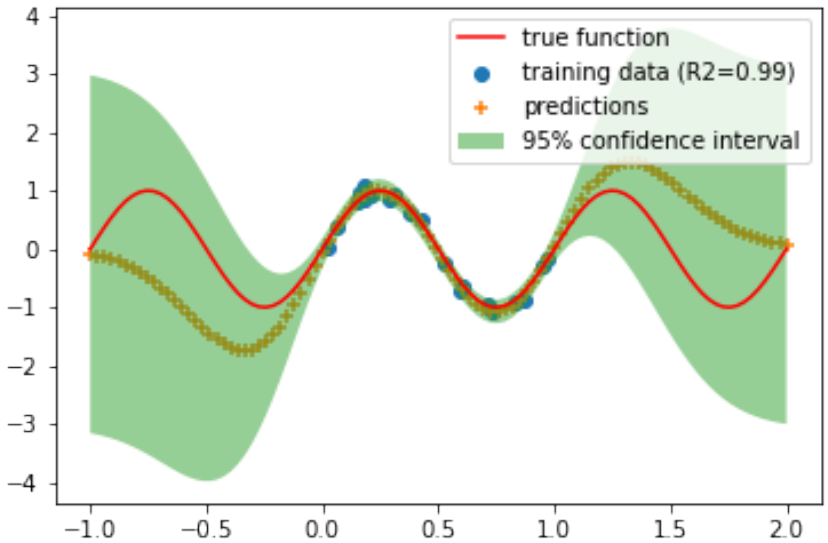
- The posterior mean function is a linear function, thus this kernel is suitable if the output is approximately linear in the features.

Squared exponential kernel

- The squared exponential kernel (aka RBF kernel) is defined as

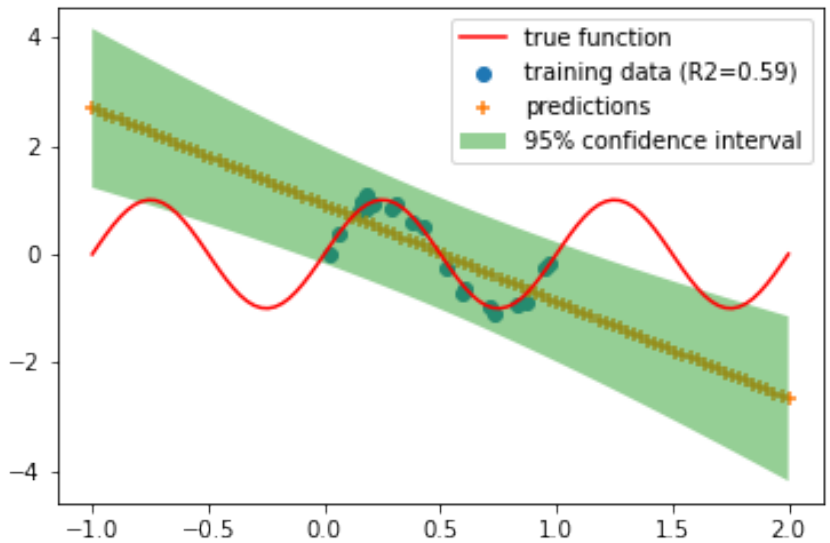
$$k_{\mathsf{SE}}(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{\|\mathbf{x} - \mathbf{x}'\|^2}{2\ell^2}\right),$$

  where ℓ is called the characteristic length scale.
- When the distance between $\mathbf{x}$ and $\mathbf{x}'$ decreases, the kernel value increases $\Rightarrow$ more similar inputs lead to more correlated outputs.



scaled RBF kernel $c \exp\left(-(\mathbf{x}-\mathbf{x}')^2/(2\ell^2)\right)$

$c = 2.435, \ell = 0.335, \sigma^2 = 0.00821$



scaled linear kernel $c(\mathbf{x}^\top \mathbf{x}' + \sigma_0^2)$

$c = 3.31, \sigma_0 = 0.509, \sigma^2 = 0.262$

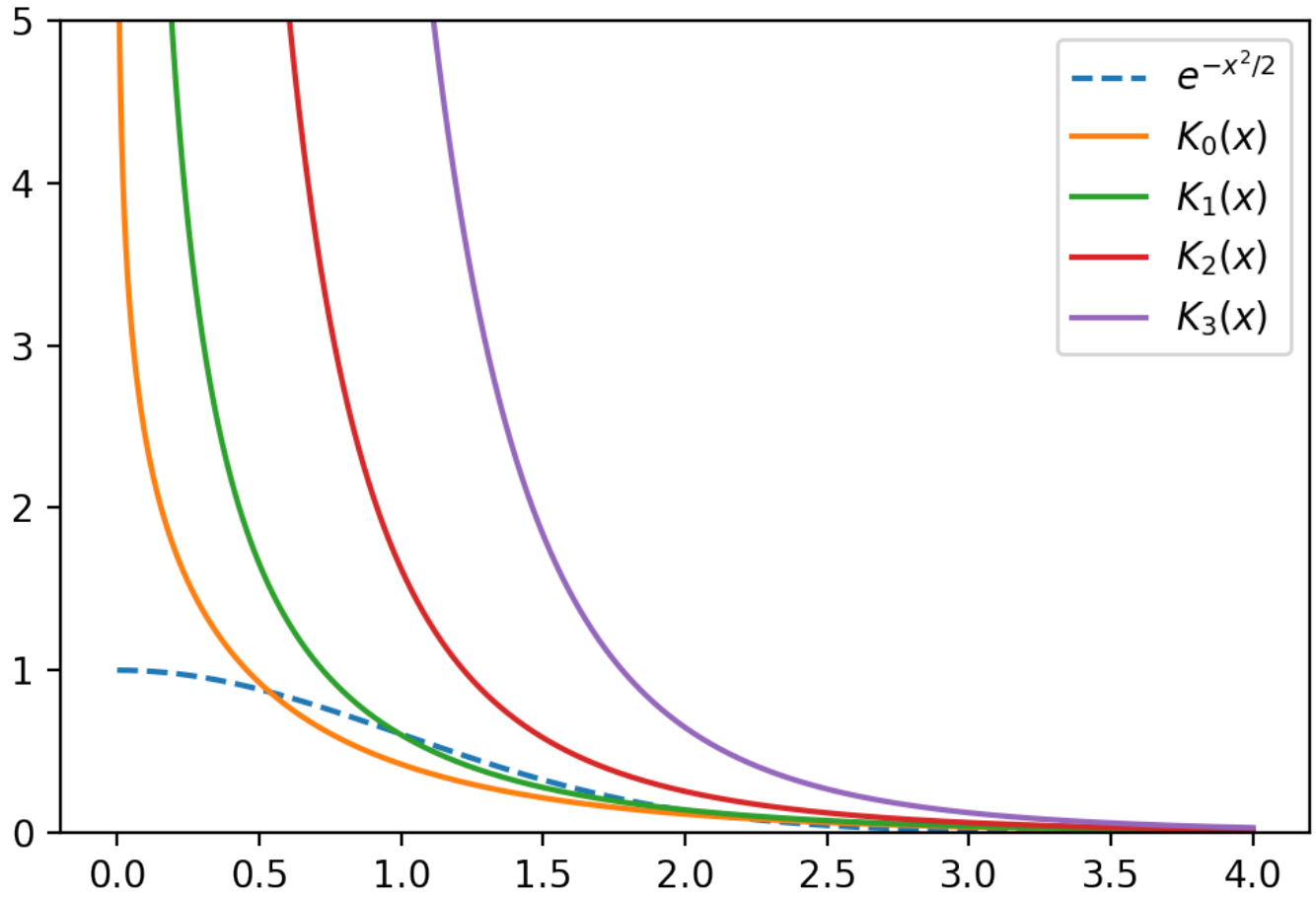
Hyperparameters in red are learned; $m = 0$.

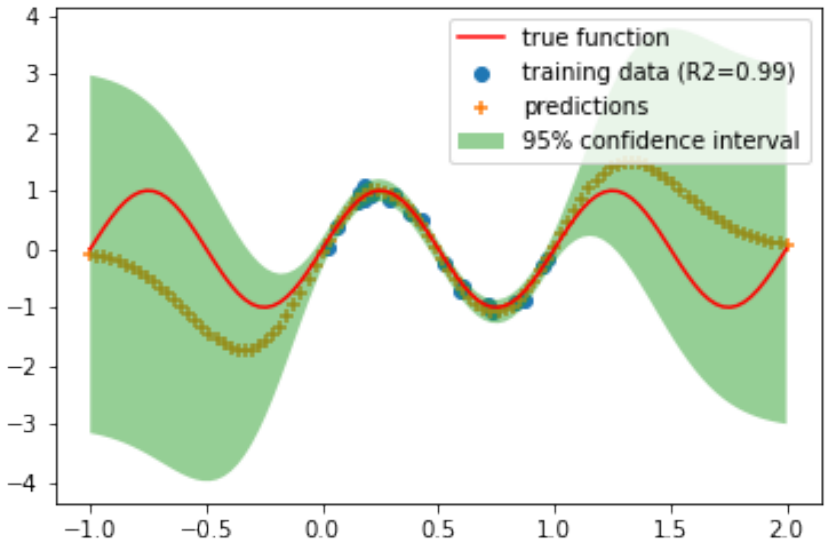
Matérn kernel

- The Matérn kernel is defined as

$$k_{\text{Matern}}(\mathbf{x}, \mathbf{x}') = \frac{2^{1-\nu}}{\Gamma(\nu)} \left(\frac{\sqrt{2\nu}\|\mathbf{x} - \mathbf{x}'\|}{\ell} \right)^{\nu} K_{\nu} \left(\frac{\sqrt{2\nu}\|\mathbf{x} - \mathbf{x}'\|}{\ell} \right),$$

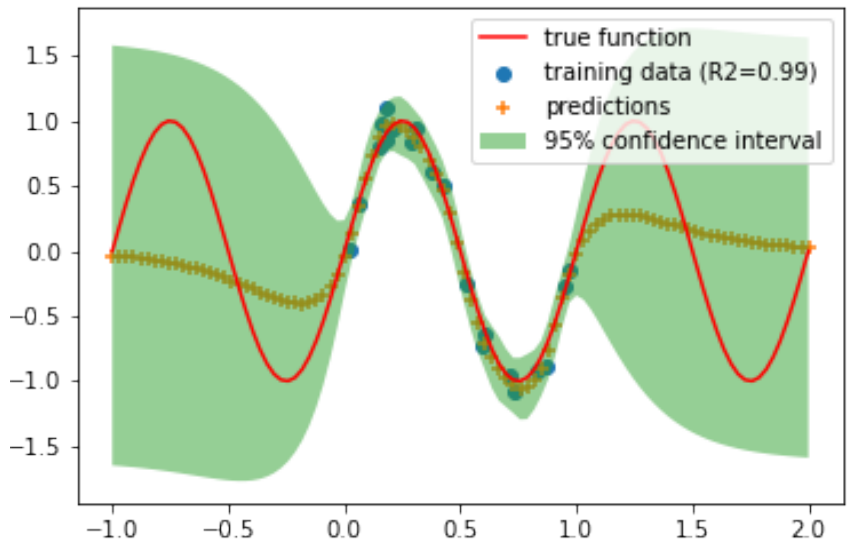
  with positive parameters ν and ℓ, where Γ is the Gamma function, and K_{ν} is the modified Bessel function of the second kind.
- $K_{\nu}(x) \sim \sqrt{\pi/(2x)} \exp(-x)$ as $x \to \infty$.


5
4
3
2
1
0
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
$e^{-x^2/2}$
$K_0(x)$
$K_1(x)$
$K_2(x)$
$K_3(x)$



scaled RBF kernel $c \exp\left(-(\mathbf{x}-\mathbf{x}')^2/(2\ell^2)\right)$

$c = 2.435, \ell = 0.335, \sigma^2 = 0.00821$



scaled Matern kernel $ck_{\text{Matern}}(\mathbf{x}, \mathbf{x}')$

$c = 0.671, \nu = 1.5, \ell = 0.344, \sigma^2 = 0.00779$

Hyperparameters in red are learned; $m = 0$.

Constructing New Kernels

- If k_1 and k_2 are kernels, then
  - $k(\mathbf{x}, \mathbf{x}') = ck_1(\mathbf{x}, \mathbf{x}')$ is a kernel for any $c > 0$.
  - $k(\mathbf{x}, \mathbf{x}') = k_1(\mathbf{x}, \mathbf{x}') + k_2(\mathbf{x}, \mathbf{x}')$ is a kernel.
  - $k(\mathbf{x}, \mathbf{x}') = k_1(\mathbf{x}, \mathbf{x}')k_2(\mathbf{x}, \mathbf{x}')$ is a kernel.
  - $k(\mathbf{x}, \mathbf{x}') = k_1(\mathbf{x}, \mathbf{x}')^p$ is a kernel.

GP Regression in sklearn

```
from sklearn.datasets import fetch_california_housing
from sklearn.gaussian_process import GaussianProcessRegressor
from sklearn.gaussian_process.kernels import WhiteKernel,
    ConstantKernel, Matern
from sklearn.model_selection import train_test_split

X, y = fetch_california_housing(return_X_y=True)
X_tr, X_ts, y_tr, y_ts = train_test_split(X, y, test_size=0.8,
    random_state=42)
# train and test a GP with scaled Matern kernel and noisy obs
kernel = ConstantKernel()*Matern()+WhiteKernel()
gpr = GaussianProcessRegressor(kernel=kernel, random_state=0)
gpr.fit(X_tr, y_tr)
print(gpr.score(X_ts, y_ts))
```

sklearn uses zero-mean GPs. By default, kernel hyperparameters are optimized during fitting.

GP Classification

- GPs can be used for classification as well.
- The theory is much more involved than that for regression and is beyond this course.
- However, there are many GP libraries, and implementing a GP classifier is easy.
- As in regression, choosing the right kernel is a main consideration in getting the most out of a GP classifier.

GP Classification in sklearn

```
from sklearn.datasets import load_digits
from sklearn.gaussian_process import GaussianProcessClassifier
from sklearn.gaussian_process.kernels import WhiteKernel,
    ConstantKernel, Matern
from sklearn.model_selection import train_test_split

X, y = load_digits(return_X_y=True)
X_tr, X_ts, y_tr, y_ts = train_test_split(X, y, test_size=0.8,
    random_state=42)
# train and test a GP with scaled Matern kernel and noisy obs
kernel = ConstantKernel()*Matern()+WhiteKernel()
gpr = GaussianProcessClassifier(kernel=kernel, random_state=0)
gpr.fit(X_tr, y_tr)
print(gpr.score(X_ts, y_ts))
```

What You Need to Know

- Bayesian learning
- Gaussian processes (GPs)
  - GPs as a generalization of multivariate Gaussians: mean function and kernel function
  - GPs as distributions on functions
  - computation of marginal distributions and conditional distributions
- GP regression
  - noisy-free and noisy observation models
  - prediction
  - model selection (maximum likelihood learning of hyperparameters)
- GP classification
- Implementing GPs in sklearn